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New Quality Indicator Statistics for the Gaseous Criteria Pollutants

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Overview

- Goals
- Review current data and statistics
- Present the new statistics
- Discussion
- Conclusions

Purpose / Goal

- The goal for this project was to develop a set of statistics that correspond to the DQO statements for the gaseous pollutants.
- The statistics need to be based on the quality indicator data already collected.
- If possible, it was desired to use statistics that would be consistent with the PM2.5 program.

The Data and Current Statistics

Pollutant	Data	Current Summary Statistic(s)
NO_2, SO_2, CO, and O_3	Biweekly Precision Checks Annual Accuracy Audits	Probability Interval Probability Interval None
Lead	Flow rate audits Lead strip audits Co-located measurements	Probability Interval Probability Interval Probability Interval
PM_{10}	Flow rate audits Co-located measurements	Probability Interval Probability Interval
$PM_{2.5}$	Flow rate audits Co-located measurements PEP measurements	Mean percent deviation from target flow. CV estimated using the Root-Mean Square of percent differences. Bias estimated by mean of percent differences.

The Probability Interval

- For the gaseous pollutants, the main quality assurance tools are the “biweekly” precision checks. The precision checks are made by sampling from air with a known concentration of a given pollutant.
- A probability interval based on the relative percent error of these checks is created. This probability interval is the main method for summarizing the relative percent errors and serves well as a summary tool.
- It does not control precision and bias separately, and these two do not contribute equally to decision errors.

"Biweekly Precision" Data

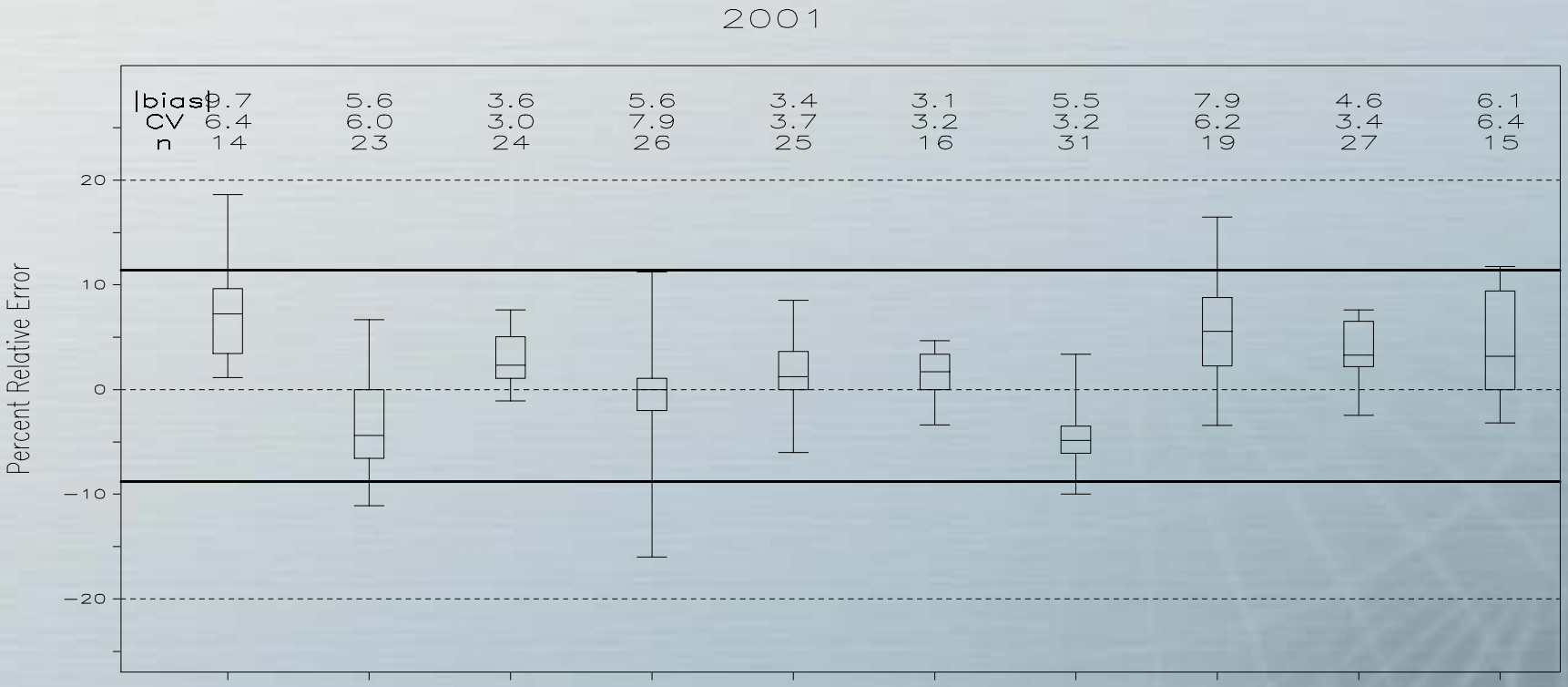
- Repeated measurements against the same "truth."
- These can be used to measure both precision and bias.
- Moreover, for automated methods they are frequently not biweekly.
- I suggest the name "Single-Point Checks".

	CO	NO_2	O_3	SO_2
Single-point check range (PPM)	**8-10**	**0.08-0.10**	**0.08-0.10**	**0.08-0.10**

Do we want to estimate?

- No! We want to control the bias and precision.
  - We do not want the best possible statistical estimates.
  - Instead we want summary statistics that let us know whether or not bias and precision are being controlled at the site level, even though the statistics are often at the reporting agency level or higher.
  - We also want to capture any season variations without allowing cancellation.

Example (Ozone 2001 Data)



The Statistics

For each single-point check, calculate the relative percent error, *d*,

$$d = \frac{ind - act}{act} \cdot 100$$

where *ind* is the concentration indicated by the agency's measurement and *act* is the actual concentration being measured.

Bias

The bias statistic is an upper bound on the mean absolute values of the relative errors.

$$\left|bias\right| = AB + t_{0.95,n-1} \cdot \frac{AS}{\sqrt{n}}$$

where:

- n is the number of single-point checks being aggregated;
- $t_{0.95,n-1}$ is the 95th quantile of a t-distribution with n-1 degrees of freedom;
- AB is the mean of the absolute values of the d's; and
- AS is the standard deviation of the absolute values.

Bias (cont.)

In particular, AB and AS are:

$$AB = \frac{1}{n} \cdot \sum_{i=1}^{n} |d_i|$$

$$AS = \sqrt{\frac{n \cdot \sum_{i=1}^{n} |d_i|^2 - \left(\sum_{i=1}^{n} |d_i| \right)^2}{n(n-1)}}$$

Precision

The precision statistic is an upper bound on the standard deviation of the relative errors.

$$CV = \sqrt{\frac{n \cdot \sum_{i=1}^{n} d_i^{\,2} - \left(\sum_{i=1}^{n} d_i \right)^2}{n(n-1)}} \cdot \sqrt{\frac{n-1}{\chi_{0.05,n-1}}}$$

where $\chi_{0.05,n-1}$ is the 5th percentile of a chi-squared distribution with n-1 degrees of freedom.

Verifying Assumptions

- The accuracy audits are annual NIST traceable audits over a range of concentrations.
- These accuracy audits can be used to verify the results obtained from the single-point checks and to validate those results across a range of concentration levels.
- Annual and three-year agency-level probability limits calculated from all the *single-point checks* should capture approximately 95 percent of the relative percent differences from the accuracy audits (for all levels).

Probability Interval

The current probability limit statistics should be kept for the single-point checks, but compared to the accuracy audits.

$$Upper\ probability\ Limit = m + 1.96 \cdot S$$

$$Lower\ probability\ Limit = m - 1.96 \cdot S$$

$$m = \frac{1}{k}\sum_{i=1}^{k} d_i \qquad S = \sqrt{\frac{k \cdot \sum_{i=1}^{k} d_i^{\,2} - \left(\sum_{i=1}^{k} d_i\right)^2}{k(k-1)}}$$

Discussion - Bias

- Since the bias is the more influential of the two types of error on decision quality, the bias is the more strongly controlled under the scheme.
- The bias statistic has two conservative components:
  - The absolute values were chosen to detect or control for cases where the bias is positive part of the time and negative part of the time.
  - The use of a confidence limit upper bound adds an additional protection, in this case, against random errors in the estimate of the mean of the absolute relative errors.
- Neither of the above is consistent with the PM2.5 program, but both are being considered for the PM2.5 program.

Discussion - Precision

- The confidence limit upper bound protects against random errors in the estimate of the standard deviation.
- The DQO quantity of interest is the CV of the measurement error, so it would not be appropriate to use the standard deviation of the absolute values as in the bias statistic.
- The statistic is less conservative than the root-mean-square statistic currently used for PM2.5, because it includes a mean correction (the second term under the first square root). This was felt to be appropriate for the gaseous pollutants.
- Moreover, the precision statistic is being considered as a replacement for the current statistic used for precision in the PM2.5 program.

Discussion - Accuracy Audits

- The accuracy audits tie everything together.
- There are not enough data from these to get summary information from them alone.
- Instead, they are consistency and assumption checks under the proposed scheme.

Conclusion

- The statistics presented make better use of the QA data currently collected by the State and Local agencies monitoring the gaseous criteria pollutants.
- They separately control the precision and bias as required by the DQO statements.
- They are not estimates of precision and bias, but rather upper bounds to control the bias and precision.
- They incorporate both the single-point check data and the accuracy audit information.